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Technical Report No. 48

Partitioning of Fibonacci Numbers
Representing Kekule Structures

by

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Prepared for Publication

in the

Journal of Mathematical Chemistry

AD-A183 887

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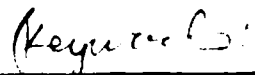Department of Chemistry
Athens, Georgia 30602

August 11, 1987

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REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER Technical Report No. 48	2. GOVT ACCESSION NO. A182887	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Partitioning of Fibonacci Numbers Representing Kekule Structures		5. TYPE OF REPORT & PERIOD COVERED Technical Report
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Sherif El-Basil		8. CONTRACT OR GRANT NUMBER(s) N00014-84-K-0365
9. PERFORMING ORGANIZATION NAME AND ADDRESS University of Georgia Department of Chemistry Athens, GA 30602		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 4007001-6
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research Department of the Navy Arlington, VA 22217		12. REPORT DATE August 11, 1987
		13. NUMBER OF PAGES 28
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office) ( )		15. SECURITY CLASS. (of this report)
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

This document has been approved for public release and sale; its distribution is unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

To be published in the Journal of Mathematical Chemistry

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Graph Theory
Factor Graphs
Fibonacci Numbers
Equivalence Relation

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

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PARTITIONING OF FIBONACCI NUMBERS

REPRESENTING KEKULE STRUCTURES

———

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ABSTRACT

When a Kekulé structure is transformed into the subspace of its double bonds a factor of graph results.[22-34] A function called <u>degenerate transformation</u> is defined on the set of factor graphs of a benzenoid system which was demonstrated to be an <u>equivalence relation.</u> For nonbranched catacondensed all-benzenoid, NBCCAB, hydrocarbons, this relation is shown to preserve the Fibonacci-type recursion of the number of their Kekulé structures.

Key words

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1. Introduction

Hosoya's two classical papers in the Fibonacci Quarterly[1,2] led for the first time to a graphical representation of Fibonacci numbers.[3] Thus Hosoya demonstrated[1,2] that the nonadjacent numbers (also defined by him[4]) of the paths are Fibonacci numbers. Thus defining[4] $p(G,k)$ to be the number of selections of k edges such that no two of them are incident an index Z is given by[4]

$$Z(G) = \sum_{k=0}^{M} p(G;k) \tag{1}$$

where M is the maximal value of k, for which $p(G,k)$ is different than zero, taking in general $p(G;o) = 1$. For a path on j vertices, L_j, Hosoya[1,2,4] discovered that

$$Z(L_j) = f_{j+1}, \qquad j \geq 2 \tag{2}$$

where f_n is an n-th Fibonacci number[3] given by $f_i = f_2 = 1$, $f_3 = 2$, $f_4 = 3$, ..., or, in general

$$f_{j+2} = f_{j+1} + f_j \tag{3}$$

Fibonacci numbers and Fibonacci-like recursions have been the focus of many recent papers of mathematical chemistry[1,2,5-11]. It has long been known that the Kekulé counts of the so called zigzag polyacenes[12] (i.e. the series phenanthrene, chrysene, picene, fulminene, ...) are Fibonacci numbers, viz.,
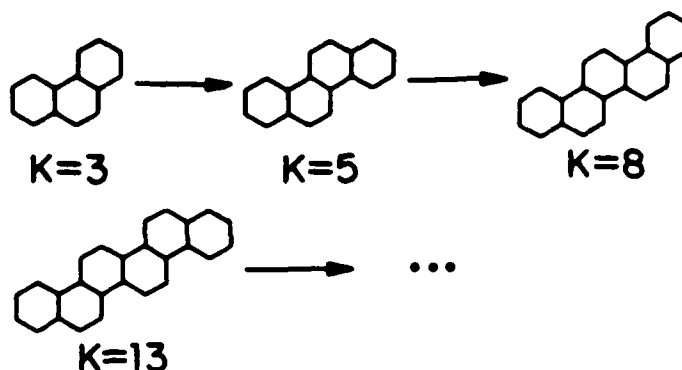
Actually this fact should now be regarded as merely "another way of stating" Hosoya's discovery which is described by Eqn. (2). In fact for any nonbranched catacondensed[13] benzenoid hydrocarbon, Gutman[14] elegantly defines a caterpillar tree,[15] T, which has the property that:

$$p(T;k) = r(B;k), \text{ for all } k = [o,M] \qquad (4)$$

where r(B;k) is the quantity introduced by Hosoya and Yamaguchi[16] and is called the kth resonant number of the benzenoid system B. It enumerates the number of ways of selecting k nonadjacent but mutually resonant rings in B. Consistently, the so called Gutman trees[14,17] of the zigzag polyacenes shown above are paths. Excluding isoconjugates, a bijective mapping[18] might be defined for:

$$\text{phenanthrene} \longrightarrow L_4, \text{ chrysene} \longrightarrow L_5, \ldots \text{ etc.}$$

In this paper we describe for the first time a partitioning of the Fibonacci numbers by decomposing a set of Kekulé structures into equivalence classes[19] such that the Fibonacci recursion, Eqn. (3) is preserved. Since we will deal with

Kekulé structures of a special kind of benzenoid hydrocarbons we state the following:
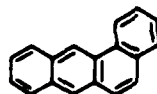
2. Definitions

2.1 An all-benzenoid system

If one of the Kekulé structures of a benzenoid hydrocarbon possesses a sextet of pi-electrons in <u>all</u> of its rings the hydrocarbon is termed <u>all-benzenoid</u>. As an illustration we consider two all-benzenoid Kekulé structures:

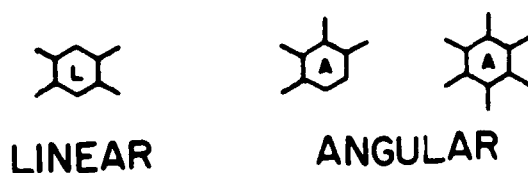and a non-all-benzenoid Kekulé structure:

There is no way of putting a 3-matchings in every ring in any of the Kekulé structures of benz[<u>a</u>]anthracene, and so it is a non-all-benzenoid system. Certainly the zigzag polyacenes are all-benzenoids.

2.2 L-A Sequence[14]

There are two ways[14,20] in which hexagons can be annelated: a linear and

an angular mode, viz.,

LINEAR   ANGULAR

The convention is then assumed that the terminal hexagons in a benzenoid hydrocarbon be labeled as L. Any non-branched catacondensed system[13] may thus be associated by an L-A sequence. Such two-letter sequences resemble the three-digit codes defined by Balaban and Harary[21] where linear annelation is given by digit 0 and kinked annelation the digits 1 or 2 for clockwise or anticlockwise kinks. The L-A sequence of a nonbranched catacondensed all-benzenoid, NBCCAB, hydrocarbon containing R rings is $LA^{R-2}L$.

2.3 Factor graph.[22-34] $F(k)$

The permutations of the double bonds form disconnected graphs. To form a connected graph a Kekulé structure is transformed into the subspace cf its double bonds. The following bijective mapping is defined: every double bond is transformed into a vertex, then two vertices v_i and v_j in $F(k)$ are connected only if their image double bonds, d_i and d_j in B are separated by a single bond. As an illustration we consider the generation of an $F(k)$

$k = k(B)$ $F(k)$ implanted in B

$F(k)$
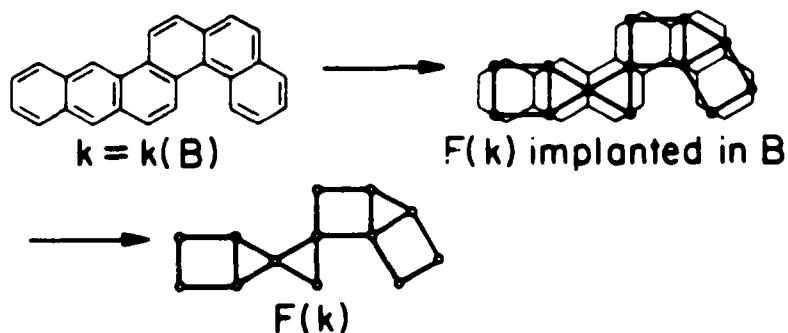
The use of factor graphs has been developed by this author[22-34] namely in the ordering of Kekulé structures, studying physical properties and understanding the topological theory of benzenoid systems. In this work one property will be considered of these objects and that is:

2.4 Degenerated Transformation

We define a transformation in a set of $F(k)$'s $\in$ B, B = a benzenoid hydrocarbon, in which an edge in $F(k_i)$ is rearranged to an adjacent vertex to generate $F(k_j)$ such that k_i, $k_j \in$ B. A degenerate transformation, thus, preserves the skeleton of the polyhex graphs. The following transformation is nondegenerate (because the parent polyhex changed from a phenanthrene to an anthracene).


Figs. 1-3 show all the degenerate transformations in the first few members of

the zigzag polyacenes (which are NBCCAB hdyrocarbons).

3. Theory

All the factor graphs considered here belong to NBCCAB systems. Investigation of Figs. 1-3 reveals that degenerate transformation, τ, partitions a set of F(k)'s of one hydrocarbon into subsets of cardinalities of 1, 2 or 4. Furthermore since in any such subsets all members are connected one might say that generates four, two or "one" cycles from a given set of F(k)'s. It turns out that the structure of the terminal cycles in an F(k) determines the cardinality of subsets. There are three basic structures, viz.,

(a) (b)

(c)
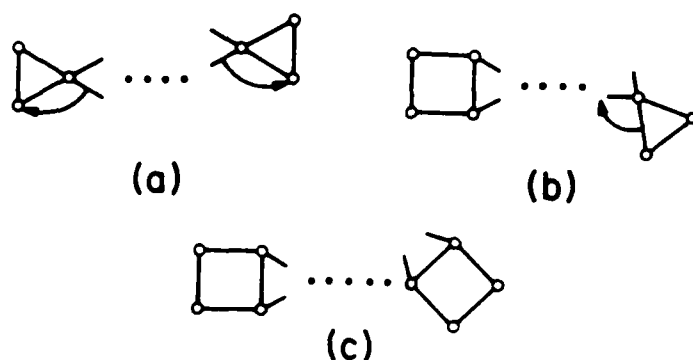
The main result of this paper depends on the following:

Lemma 1

A degenerate transformation τ partitions a set of factor graphs, $\{F(k)\}\epsilon$ NBCCAB system into four-, two- and/or one-cycles only. No other cycles are possible.

Proof   See Corollary 2.

Lemma 2

Let $|<4>|$ be the number of 4-cycles i.e. the number of quartets of $F(k)$'s linked by a τ and similarly for $|<2>|$ and $|<1>|$. If $|(a)|$ = the number of $F(k)$'s of type (a) etc., then

$$|<4>| = |(a)|$$
$$|<2>| = |(b)| \tag{5}$$
$$|<1>| = |(c)|.$$

Proof

It can be seen from Figs. 1-3 that any <u>terminal</u> C_3 (i.e. a 3-cycle) in an $F(k)$ can undergo a τ to give another $F(k)$ <u>with a terminal C_3 also.</u> So an $F(k_1)$ of type (a) generates $F(k)_2$ and $F(k_3)$ (each with 2 terminal C_3's). Both $F(k_2)$ and $F(k_3)$ are linked to other $F(k)$'s namely $F(k_1)$ and $F(k_4)$. Since the latter contains also two terminal C_3's it is linked to $F(k_2)$ and $F(k_3)$ and so the general form of a $<4>$ is:

$$
\begin{array}{ccc}
 & F(k_1) & \\
F(k_3) & & F(k_2) \\
 & F(k_4) &
\end{array}
$$
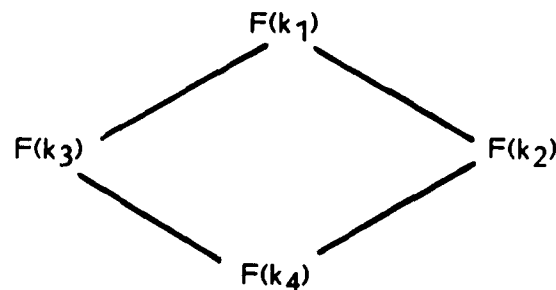
In case of type (b) it can undergo a τ to only one other $F(k)$, since a terminal

square, i.e. C_4, cannot undergo a transformation that preserves the topology of B. For example we consider the following F(k):

Topology Not Conserved

It should now be obvious that an F(k) of type (c) with two terminal C_4's simply cannot undergo a degenerate transformation and hence the number of such F(k)'s will be the number of "lonely" F(k)'s i.e. $| <1> |$.

The above two Lemmas lead to:

Theorem 1

A degenerate transformation τ partitions a set $\{F(k)\}$ into equivalence classes[19] i.e. τ is an equivalence relation.

Proof

The theorem will be proved for the four-cycles only since in a two-cycle the reflexive and symmetric parts are obvious (i.e., every factor graph is related to itself and any two F(k)'s can be related either by a τ or a τ^{-1}).

In any four-cycle all the F(k)'s have two terminal triangles and thus two degenerate transformations are possible, viz., τ_α and τ_β which can take place at either of the termini of any of the four F(k)'s of the $<4>$. Then any two F(k)'s

ϵ <4> can be related by one of the following functions: τ_α, τ_β, τ_α^{-1}, τ_β^{-1}, $(\tau_\alpha + \tau_\beta)$, $(\tau_\alpha^{-1} + \tau_\beta)$, $(\tau_\alpha + \tau_\beta^{-1})$, or $(\tau_\alpha^{-1} + \tau_\beta^{-1})$. The digraph of Fig. 4 illustrates these functions for an arbitrary <4>. Obviously any two F(k)'s which are related by either τ_α, τ_β or their inverses will occupy adjacent points on the cycles while other functions relate nonadjacent F(k)'s. This demonstrates clearly the symmetric part of the equivalence relation. Similarly the transitive part can be seen: suppose any arbitrary three F(k)'s, $F(k)_1$, $F(k)_2$ and $F(k)_3$ and let $f_1 (F(k)_1) = F(k)_2$; $f_2(F(k)_2) = F(k)_3$ where f_1, f_2 are any of the τ functions listed above then $(f_1 + f_2)(F(k)_1) = F(k)_3$. Hence τ is an equivalence relation.

Now we state the main result of this paper as:
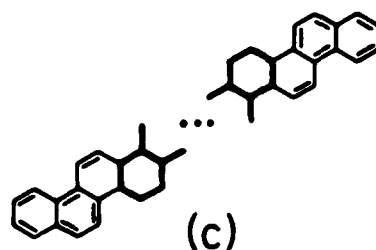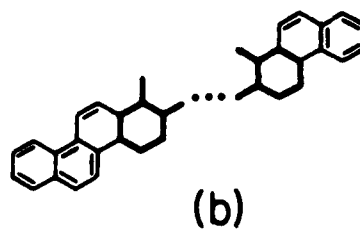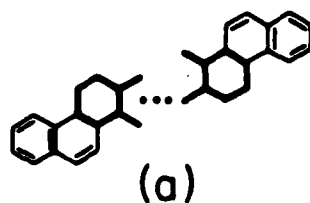
Theorem 2

Let $K(R_j)$ be the number of Kekulé structures in an NBCCAB hydrocarbon containing j rings. Let $\vdash\{K(R_j)\}$ be the partition induced on $K(R_j)$ by the function τ, then

$$\vdash\{K(R_j)\} \ \cup \vdash\{K(R_{j+1})\} \ = \vdash\{K(R_{j+2})\} \tag{6}$$

Eqns. (6) and (3) are, of course, isomorphic.

Proof

We use Lemma 2 (Eqns. 5). Namely, the individual valence-bond structures that correspond to F(k)'s of types (a), (b) and (c) are shown below:

(a)

(b)

(c)

The populations of (a), (b), (c), i.e. $|(a)|$, $|(b)|$, $|(c)|$ in a given set $\{F(k)\}$ determines the numbers $|<4>|$, $|<2>|$ and $|<1>|$ respectively.

Let the hexagons of the NBCCAB system, which we will abbreviate as B, be labeled $h_1, h_2, ..., h_{j-1} h_j$, j being the number of hexagons in B. Further, $B \ominus \{h_k h_\ell h_m ...\}$ is the benzenoid system obtained when the set of rings plus all edges incident to it is pruned out of B. Then we have the following identities:

$$|(a)_j| = K(B \ominus \{h_1 h_j\}) \tag{7}$$

$$|(b)_j| = K(B \ominus \{h_1 h_{j-1} h_j\}) \tag{8}$$

$$|(c)_j| = K(B\theta\{h_1 h_2 h_{j-1} h_j\}) \tag{9}$$

where $|(a)_j|$ is the number of Kekulé structures of type (a) for a hydrocarbon B containing j rings, and similarly for other symbols.

Now because of Eqn. (3) we can write

$$|(a)_j| + |(a)_{j+1}| = |(a)_{j+2}| \tag{10}$$

Similar equations can be written for $|(b)_j|$ and $|(c)_j|$ and having in mind Lemma 2 we have

$$|<4>_j| + |<4>_{j+1}| = |<4>_{j+2}| , \tag{11}$$

$$|<2>_j| + |<2>_{j+1}| = |<2>_{j+2}| , \tag{12}$$

$$|<1>_j| + |<1>_{j+1}| = |<1>_{j+2}| \tag{13}$$

Now, since

$$|<4>_j| + |<2>_j| + |<1>_j| = K(B_j) \tag{14}$$

theorem 2 is proved.

Corollary 1

$$R(\text{number of rings}) = 3 \iff |<2>| = 0 \tag{15}$$

$$R = 4 \Longleftrightarrow | <1> | = 0 \qquad (16)$$

Corollary 2

Since hydrocarbons for which R = 3, R = 4 has __only__ cycles of type <1>, <2> and <4> then theorem 2 leads immediately to Lemma 1 (which was stated at the beginning only for clarification).

Table 1 contains partitions of the Kekulé structures (which represent Fibonacci numbers) of the first few members of the zigzag polyacenes.

Corollary 3

Let the partition of a set of Kekulé structures of an NBCCAB hydrocarbon containing j rings be expressed as { $<1>^r$ $<2>^s$ $<4>^t$ } where $<1>^r$ means that <1> occurs r times etc. Then it follows from theorem 2 and the partitions of the first two members, (Table 1), that $r + s + t = f_j$; the __jth__ Fibonacci number.

4. Discussion of Theory

In this paper we have given for the first time a rigorous difinition for degenerate transformation on a set of Kekulé structures. The concept has been found useful in the ordering of Kekulé structures.[34] The function τ might be illustrated as follows

$$\{K\} \xrightarrow{\quad \tau \quad} \{C\} \qquad (17)$$

where { K } is a set of Kekulé structures and {C} is a set of cycles the vertices

of which represents individual factor graphs linked by τ. If we consider a homologous series of NBCCAB hydrocarbons the above mapping might be pictorially illustrated by

$$\{K\}_i \xrightarrow{\ \tau\ } \{C\}_i$$

(18)

$$\{K\}_{i+1} \xrightarrow{\ \tau\ } \{C\}_{i+1}$$

where $\{K\}_i$ is a set of Kekulé structures of a hydrocarbon containing i rings and so on. The operation in the set $\{K\}$ is <u>addition</u> recursively as given by Eqn. (3) while the operation in $\{C\}$ is <u>union</u> as described by Eqn. (6). The function τ partitions $\{K\}$ into the set $\{C\}$ of disjoint cycles so that it preserves the recursion given by Eqn. (3), namely if one considers phenanthrene to be the leading hydrocarbon, we can illustrate the τ function as follows:

$$\tau : 5 \longrightarrow \{1 + 4\}$$

$$\tau : 8 \longrightarrow \{2 + 2 + 4\}$$

$$\tau : 13 \longrightarrow \{1 + 2 + 2 + 4 + 4\}$$

$$\vdots \qquad\qquad \vdots$$

Stated formally, one can write:

$$\tau (f_i \cdot f_{i+1}) = \tau(f_i) \cdot \tau(f_{i+1})$$

(19)

where f_i is the number of Kekulé structures in the NBCCAB system whose number of rings is i-1.

5. Possible Chemical Applications

Benzenoid hydrocarbons continue to be of considerable interest both theoretically and experimentally. Two theoretical tools have been so far used to study them, viz., molecular orbital approaches and valence-bond methods. The latter involve the use of Kekulé structures either as such or in their Clar formulas.[35] Recently Herndon and Hosoya[36] used special Kekulé structures which correspond to maximal independent sets[37] of Clar structures as a base set in a valence-bond Hamiltonian and reproduced Dewar-de Llano resonance energies.[38] Factor graphs, studied in this work represent a special form of connected graphs representing the permutations of the double bonds in the individual Kekulé valence-bond structures. Factor graphs have been used to study[39-41] the sextet polynomial,[16] to order Kekulé structures[22-34] and to study the physical properties of benzenoid hydrocarbons.[42] As an illustration we consider the partitioning of the Kekulé structures of the 5-ring zigzag system: The equivalence relation τ partitions this set of Kekulé structures into two four-cycles, two two-cycles and a one "1-cycle". The two four-cycles and the corresponding conjugated circuits[43] are shown in Fig. 5. It is clear that the individual cycles lead to ordering of these circuits. The partial sums of the circuits are shown in parentheses below structures. For example the Kekulé structure possessing $3R_1 + 2R_3 + R_5$ is associated with the code (3, 0, 2, 0, 1), i.e. $3R_1$, $0R_2$, $2R_3$, $0R_4$, R_5 and therefore its partial sum would be (3, 3, 5, 5, 6). The τ function leads to partial sums satisfying Muirhead's theorem of ordering.[44] Another possible chemical application of degenerate transformations could be in the calculation of resonance energies of large molecules. One Kekulé structure is chosen from each equivalence class, in this way the number of Kekulé structures that one has to deal with is very much reduced. This approach compares with a recent statistical method advocated

by Randić[45] for the computation of resonance energies of large molecules by randomly selecting a small number of Kekulé structures from the total set. Here we suggest to use equivalence to mean a "lower form of equality" and thus to obtain a _selected_ number of Kekulé structures one does not have to draw all Kekulé structures but instead draw only those Kekulé structures which represent types (a), (b) and (c) of the factor graphs. Work in this direction is in progress.

Acknowledgments

Table 1

Partitions of Kekulé structures of NBCCAB systems induced by degenerate transformation. $(<i>)^n$ is a cycle of i factor graphs repeated n times. Observe that the sum of exponents for a system containing j rings is the jth Fibonacci number.

Number of rings	Partition
3	$<1>$, $<4>$
4	$(<2>)^2$, $<4>$
5	$<1>$, $(<2>)^2$, $(<4>)^2$
6	$<1>$, $(<2>)^4$, $(<4>)^3$
7	$(<1>)^2$, $(<2>)^6$, $(<4>)^5$
8	$(<1>)^3$, $(<2>)^{10}$, $(<4>)^8$
9	$(<1>)^5$, $(<2>)^{16}$, $(<4>)^{13}$

in general:

$j\ (\geq 5)$	$(<1>)^a$, $(<2>)^b$, $(<4>)^c$
$j+1$	$(<1>)^{a'}$, $(<2>)^{b'}$, $(<4>)^{c'}$
$j+2$	$(<1>)^{a+a'}$, $(<2>)^{b+b'}$, $(<4>)^{c+c'}$

Fig. Legends

Fig. 1

Degenerate transformation on the set of factor graphs of phenanthrene. The individual factor graphs are boldly outlined and embedded into their polyhex graphs (for convenience). The set is partitioned into two disjoint cycles: a 4-cycle, <4>, and a 1-cycle, <1>.

Fig. 2

Partitioning of the set of factor graphs of chrysene by degenerate transformations into a four-cycle and two disjoint 2-cycles.

Fig. 3

Partitioning of the factor graphs of an all-benzenoid nonbranched catacondensed hydrocarbon containing five rings by degenerate transformations into five equivalence classes, viz., two 4-cycles, two 2-cycles and a "lonely" factor graph.

Fig. 4

Pictorial illustration of the equivalence relation of theorem 1. The digraph shows paths from any factor graph to another by either a single τ or a combination of two τ functions which demonstrates both symmetric and transitive characters.

Fig. 5

Illustration of the ordering of Kekulé structures representing the factor graphs of a four cycle. The partial sums of the conjugated circuits are written in parentheses.
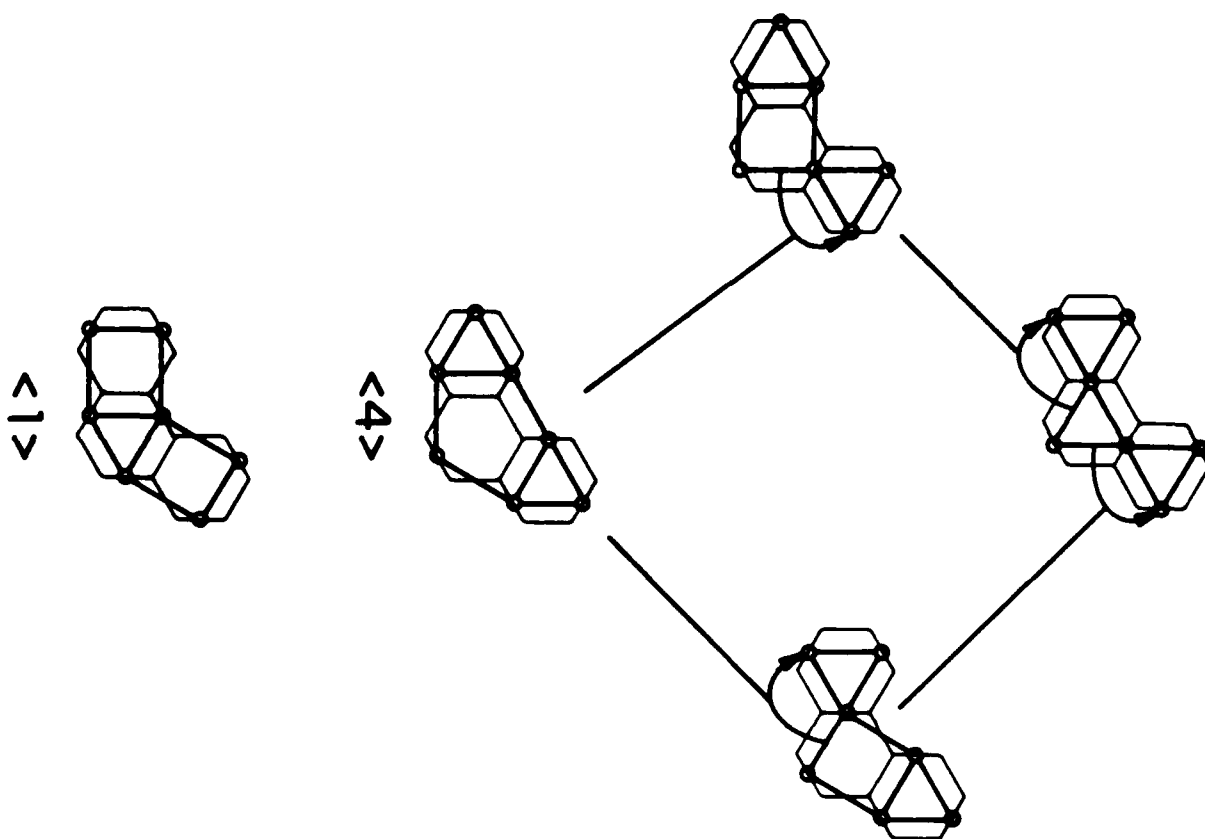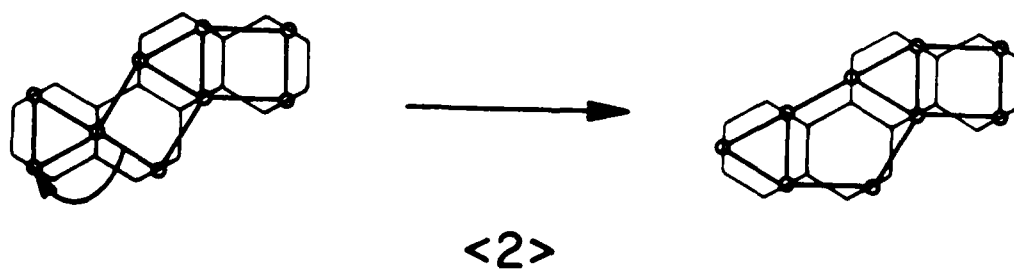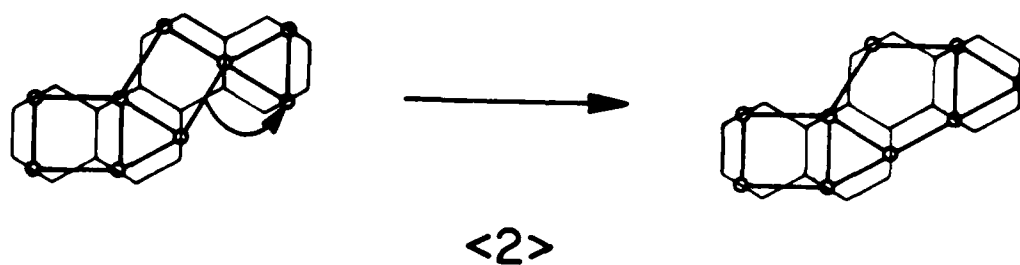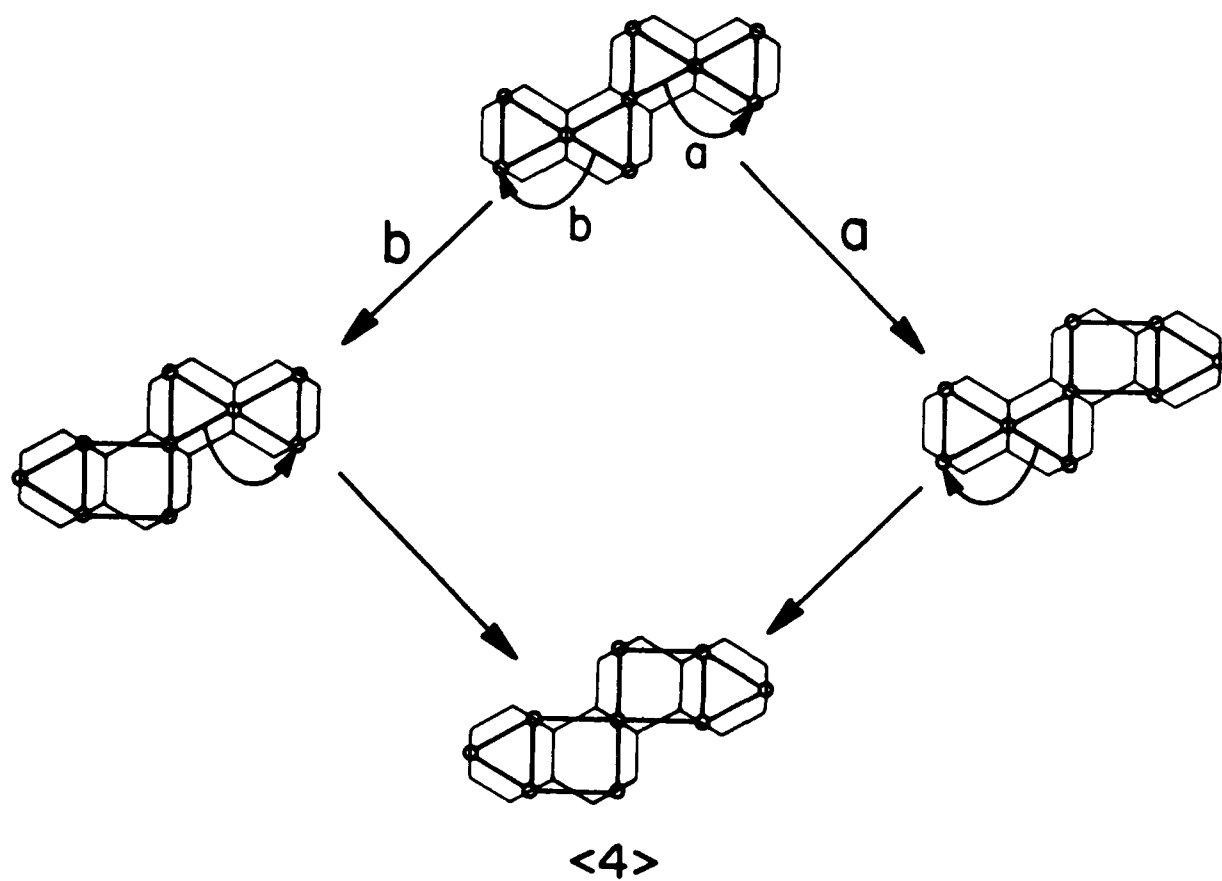
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(18) Bijective mapping is defined in: C.L. Liu, Elements of Discrete Mathematics (McGraw-Hill 1977).

(19) See Ref. 18. p. 72.

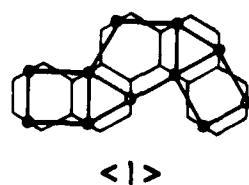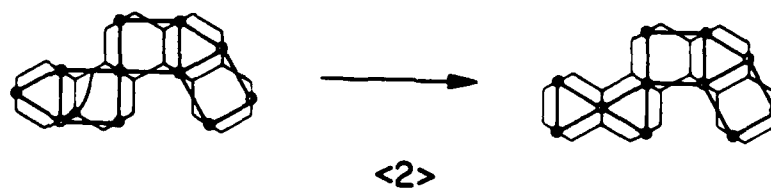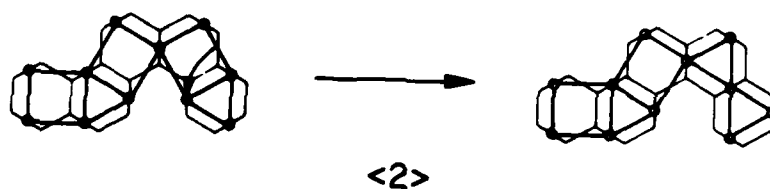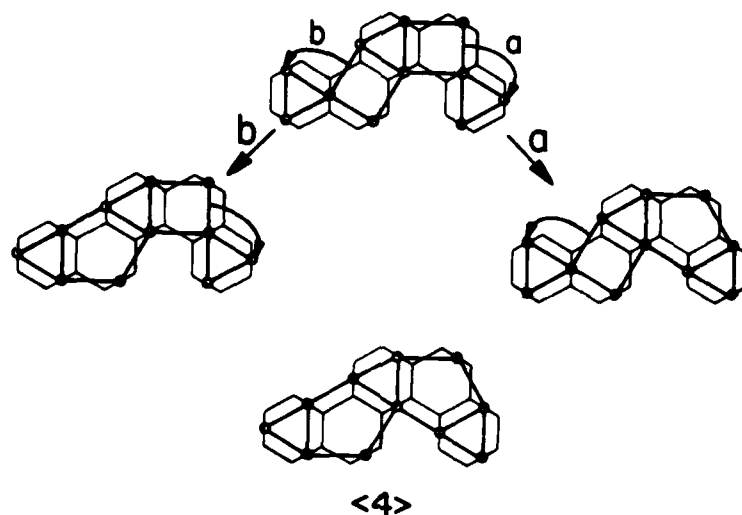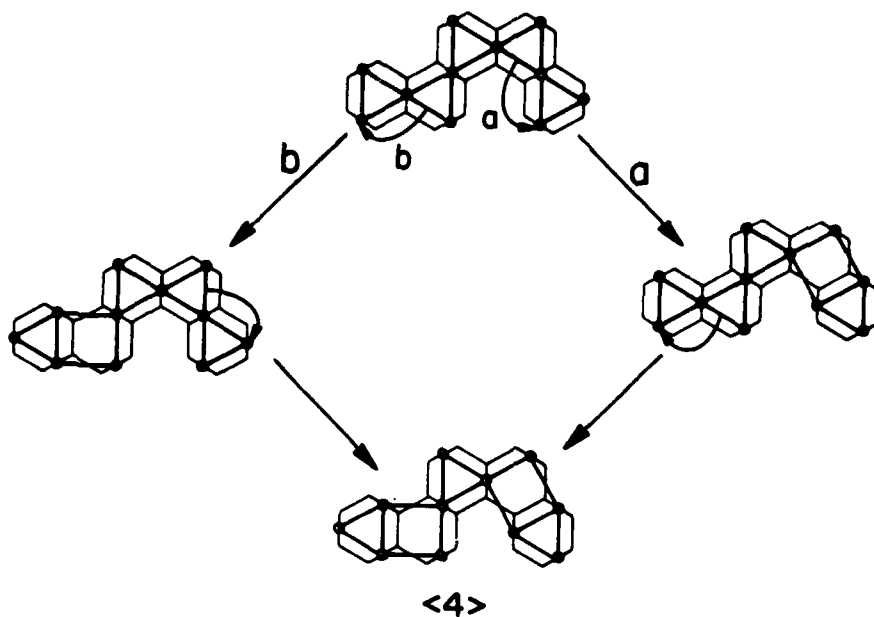(20) I. Gutman and S. El-Basil, Z. Naturforsch 39a, 276 (1984).

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(37) An independent set of vertices V(r) is said to be a maximal set if every vertex of the graph not included in V(r) is adjacent to at least one of the r vertices of V(r), c.f., N. Christofides, "Graph Theory, An Algorithmic Approach," Academic Press, New York (1975) Chapt. 3.

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<4>

<2>

<2>

<4>

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<2>

<2>

<1>

Fig 3

$$\left(\tau_\beta^{-1} + \tau_a\right)$$

$$\tau_\beta \qquad \tau_a$$

$$\tau_\beta^{-1} \qquad \tau_a^{-1}$$

$$\left(\tau_a + \tau_\beta\right) \qquad \left(\tau_a^{-1} + \tau_\beta^{-1}\right)$$

$$\tau_a^{-1} \qquad \tau_\beta^{-1}$$

$$\tau_a \qquad \tau_\beta$$

$$\left(\tau_a^{-1} + \tau_\beta\right)$$

$3R_1 + 2R_2 + R_3$
$(3,5,6,6,6)$

$3R_1 + R_2 + R_3 + R_4$
$(3,4,5,6,6)$

$3R_1 + R_2 + R_3 + R_4$
$(3,4,5,6,6)$

$3R_1 + 2R_3 + R_5$
$(3,3,5,5,6)$

$5R_1$
$(5,5)$

$4R_1 + R_2$
$(4,5)$

$4R_1 + R_2$
$(4,5)$

$3R_1 + 2R_2$
$(3,5)$

Fig 5

END

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DTIC